

1,2,3-Trichloropropene
96-19-5 | DTXSID3047766

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.92

Global applicability domain: Inside

Local applicability domain index: 6.82e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

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1,1,1-Trichloroethane

Measured: 5.01

Predicted: 7.56

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1,1,2-Trichloroethane

Measured: 5.01

Predicted: 6.36

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3,4-Dichloro-1-butene

Measured: 12.9

Predicted: 10.1

Image not found

Trichloroethylene

Measured: 15.8

Predicted: 15.2

Image not found

1,1-Dichloroethylene

Measured: 12.9

Predicted: 9.95